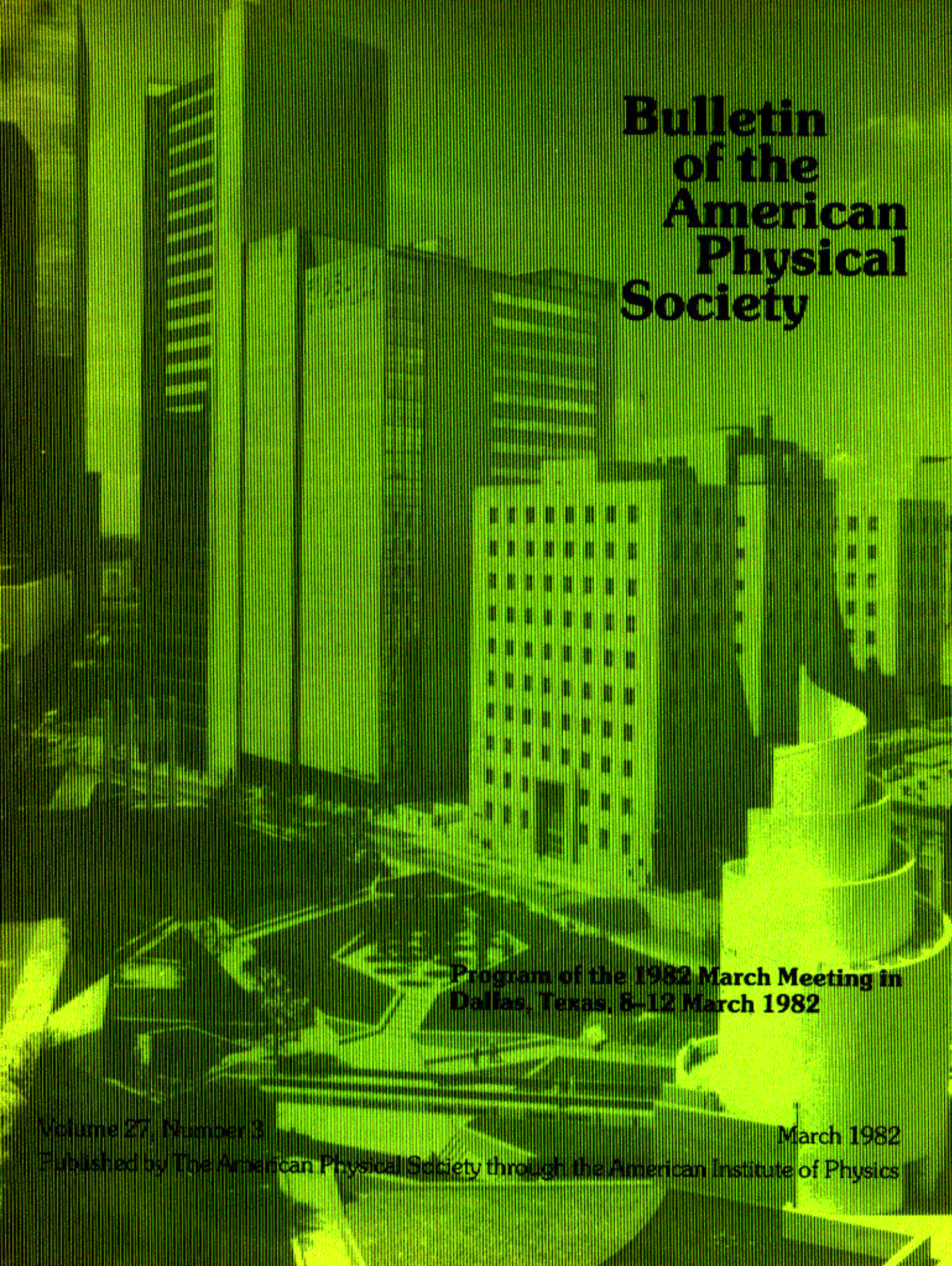


Bulletin of the American Physical Society

Program of the 1982 March Meeting in Dallas, Texas, 8–12 March 1982

Volume 27, Number 3

March 1982

Published by The American Physical Society through the American Institute of Physics

method of producing bare transition metal clusters in the gas phase. The feasibility of this technique is illustrated by the results of its application to the generation of Co_2 from $Co_2(CO)_8$. Given the diversity of known potential precursors, this technique is expected to provide specific access to a wide variety of bare transition metal clusters.

KO 6 Excitation of Multi-Level Systems by a Quasimonochromatic Field of Time-Varying Intensity. R. S. BURKEY and C. D. CANTRELL, U. of Texas at Dallas--We calculate the population and dipole-moment expectation value of multi-level, nearly degenerate systems irradiated by a pulsed, quasimonochromatic laser field. The calculations described include an analytic solution in the case of an exponentially varying field amplitude, and a numerical integration in the case of a general time variation; neither technique requires use of the adiabatic-following approximation. Level structures of systems for which plots of populations and polarization versus time, laser frequency, and field strength are presented include one or more nondegenerate levels radiatively coupled to one or more "bands" of nearly degenerate levels.

KO 7 Refractive Index of Nearly Degenerate Multilevel Systems in a Monochromatic Field. G. L. PETERSON, R. S. BURKEY, and C. D. CANTRELL, U. of Texas at Dallas.--We report calculations of the index of refraction (n) and populations of energy levels in several different multilevel systems, under the influence of a monochromatic field in the adiabatic-following approximation. These systems include: (1) a single lower level and several nearly degenerate upper levels with transitions allowed only between the lower and upper levels; (2) two nondegenerate lower levels and several nearly degenerate upper levels with transitions allowed only between the two single levels, and between the higher single level and the several nearly degenerate upper levels; (3) the same system as (2) but with the higher single level replaced by several nearly degenerate levels. Plots of n-1 versus frequency and field strength, along with plots of level populations versus field strength, are presented for all systems. Results will be shown for finite and infinite population and coherence decay times.

KO 8 Role of the Anderson Transition in Electronic Energy Transfer in Mixed Organic Crystals, J. KLAFTER, C. M. SOUKOULIS and E. N. ECONOMOU*, Corporate Research Science Laboratories, Exxon Research and Engineering Co., Linden, N.J. 07036 - We have analyzed some recent experimental data on triplet electronic energy transfer (EET) in isotopically mixed naphthalene. These data give the efficiency of EET as a function of an energy sink concentration. We have advanced a possible interpretation of these results in terms of the gradual growth of the participation ratio above the transition concentration $\bar{c}$. Such a behavior at $\bar{c}$ reflects the same features of the eigenfunctions responsible for the continuous behavior of the mobility at the mobility edges. A coherent potential approximation is used to calculate averaged Green's functions; the L(E) criterion is employed to study the transition in the nature of the eigenstates. The transition is found to take place at a concentraiton $\bar{c}$, which is qualitatively in agreement with experiments.

*Dept. of Physics, University of Crete, Iraklion, Crete, Greece.

KO 9 Inner Shell Ionization Cross section for Argon, Krypton and Xenon. Carroll Quarles, Mars Semaan and Lee Estep, Texas Christian U.--As part of experiment to measure atomic-field bremsstrahlung from the electron bombardment of thin rare gas targets in the electron energy range of 1-10 keV, we have measured the K-shell ionization cross section for argon and the L-shell ionization cross section for krypton and xenon in this same electron energy range. Preliminary results will be presented for the absolute cross section obtained by normalizing to the theoretical bremsstrahlung cross section, and will be compared with other experimental work in this energy range as well as with the results of various theoretical calculations for the inner shell ionization cross section.

KO 10 Magnetic Dipole Transition Amplitude M_1 for $6P_{\frac{1}{2}} \rightarrow 7P_{\frac{1}{2}}$ Transition in Atomic Thallium. B.P. DAS and T.P. DAS, SUNY Albany, J. ANDRIESSEN, Technische Hogeschool Delft, Netherlands, TAESUL LEE, Computer Science Corporation, Silver Springs, Maryland and S.N. RAY, Systems and Applied Sciences Corporation, Riverdale, Maryland.—Using relativistic many-body theory, we have calculated the magnetic dipole transition amplitude M_1 for the $6P_{\frac{1}{2}} \rightarrow 7P_{\frac{1}{2}}$ transition in atomic thallium, which is important for the understanding of the theory of the circular dichroism effects in thallium atom due to the presence of the parity-violating neutral weak current interaction. Our net result for M_1 is $-2.43 \times 10^{-5} \mu_B$ which is in satisfactory agreement with the experimental value[1] of $(-2.11 \pm 0.30) \times 10^{-5} \mu_B$. The net theoretical result is composed of -1.500, 0.032 and $-0.957 \times 10^{-5} \mu_B$ from direct, consistency and correlation effects. Physical reasons for the relative importance of these effects will be discussed.
[1]S. Chu, E.D. Commins and R. Conti Phys. Lett. 60A, 96 (1977)

KO 11 Theory of Hyperfine Interactions in Alkaline Earth Ions - $^{25}Mg^+$. S. AHMAD AND T.P. DAS, SUNY Albany and J. ANDRIESSEN, Technische Hogeschool Delft, Netherlands*. Relativistic many-body perturbation theory[1] has been used to investigate the hyperfine structure of singly ionized magnesium ion, to explain the recent experimental data[2] on Mg^+ as well as to compare the results in alkali atoms with those in the corresponding isoelectronic alkaline-earth positive ion series. The one-electron contribution to the hyperfine constant in $^{25}Mg^+$ was found to be -553 MHz, composed of direct and exchange core polarization contributions of -466 MHz and -87 MHz respectively, the many-electron contribution being -48 MHz. The net theoretical hyperfine constant comes out as $-(602 \pm 8)$ MHz, in good agreement with the experimental value[2] of -596.25 MHz.
*Supported by NIH grant GM25230
[1]M. Vajed-Samii, et.al. Phys. Rev. A 20, 1787 (1979).
[2]W.M. Itano and D.J. Wineland, Phys. Rev. A 24, 1364 (1981).

Supplemental Program

KO 12 Relativistic Theory of Hyperfine Interactions in Excited $^2S_{\frac{1}{2}}$ States of $^{137}Ba^+$ Ion*. S. AHMAD, T.P. DAS, SUNY Albany and J. ANDRIESSEN, Technische Hogeschool Delft, Netherlands.—Using relativistic many-body perturbation theory, we have investigated the mechanisms contributing to the hyperfine interaction in excited $^2S_{\frac{1}{2}}$ states (7s through 11s) of $^{137}Ba^+$ ion. In addition to showing a rapid decrease in the net hyperfine constants in going to higher states, the results show interesting features for the ratio of the exchange core polarization and correlation contributions to the direct contribution, some of them being distinct from the trends in neutral alkali atoms[1]. The ECP

EXCITATION OF MULTI-LEVEL SYSTEMS BY A QUASI-MONOCHROMATIC FIELD OF TIME-VARYING INTENSITY

R.S. BURKEY AND C.D. CANTRELL
UNIVERSITY OF TEXAS AT DALLAS

RESEARCH SUPPORTED BY
NSF GRANT NO. CHE-8017324

THE EXPONENTIAL PULSE SOLUTION (EPS)

SCHRÖDINGER EQUATION FOR A MULTI-LEVEL SYSTEM INTERACTING WITH A CLASSICAL ELECTRIC FIELD:

$$\frac{d}{dt}\,v = i\,\delta\,v + i\,\epsilon(t)\,\mu\,v$$

- v: STATE VECTOR
- δ: DIAGONAL MATRIX OF UNPERTURBED ENERGIES
- $\epsilon(t)$: FIELD
- μ: MATRIX OF ELECTRIC DIPOLE

[IF THE FIELD IS QUASI-MONOCHROMATIC, WE CAN USE THE ROTATING-WAVE APPROXIMATION TO GET AN EQUATION OF THIS FORM, BUT IN WHICH $\epsilon(t)$ IS THE PULSE ENVELOPE AND δ CONTAINS DETUNINGS.]

USE THE PULSE-AREA $\tau = \int_{-\infty}^{t} \epsilon(\lambda)\,d\lambda$ AS A "TIME" VARIABLE:

$$(*) \qquad \frac{d}{d\tau}\,v(\tau) = \frac{i}{\epsilon(\tau)}\,\delta\,v(\tau) + i\mu\,v(\tau) \quad .$$

FOR SPECIAL PULSE SHAPES $\epsilon(\tau)$, EQUATION (*) CAN BE SOLVED. WITHOUT LOSS OF GENERALITY, WE ASSUME THE INITIAL CONDITION

$$v\big|_{t=-\infty} = v\big|_{\tau=0} = \text{GROUND STATE} \quad .$$

WE HAVE FOUND ESPECIALLY INTERESTING SOLUTIONS FOR TWO PULSE SHAPES:

1) $\epsilon(\tau) = \lambda\tau$, WHICH IMPLIES THAT $\epsilon(t) = \epsilon_0 e^{\lambda t}$, GIVES THE "EXPONENTIAL PULSE SOLUTION" (EPS);

2) $\epsilon(\tau) = \frac{\lambda\tau}{1 + \frac{\lambda}{\epsilon_\infty}\tau}$, WHICH INITIALLY INCREASES EXPONENTIALLY BUT EVENTUALLY GOES TO THE FIXED VALUE ϵ_∞, GIVES THE "SEMI-EXPONENTIAL PULSE SOLUTION" (SEPS).

THE EPS IS A LIMITING CASE OF THE SEPS WHEN $\epsilon_\infty \to \infty$.

WITH THESE PULSE SHAPES, SERIES SOLUTIONS FOR EQUATION (*) CAN IMMEDIATELY BE WRITTEN:

$$(**) \quad v(\tau) = \sum_{k=0}^{\infty} \underset{\text{VECTOR COEFFICIENT}}{v_k} \tau^k ,$$

WHERE

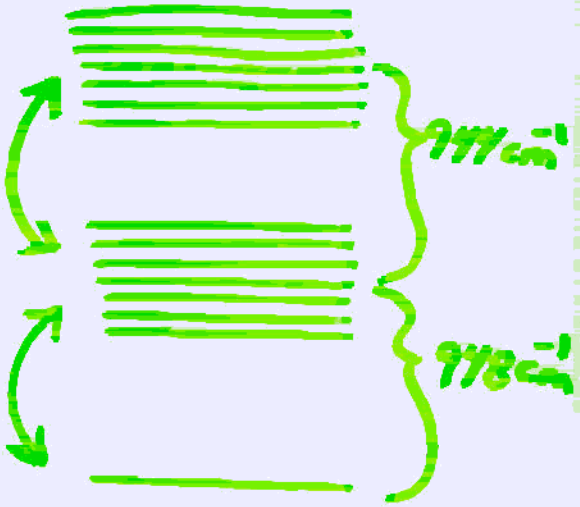
$$v_0 = v\big|_{\tau=0}$$

AND

$$v_{k+1} = i\left(k+1 - \frac{i}{\lambda}\delta\right)^{-1}\left(\mu + \frac{1}{\epsilon_\infty}\delta\right)v_k .$$

THE SEPS CONVERGES ANALYTICALLY FOR ALL τ. THE REGION OF PRACTICAL CONVERGENCE IS, OF COURSE, FINITE. (IN THE EPS CASE, WE

BELIEVE THAT THIS REGION IS $0 \leq E(t) < \frac{2\pi}{\mu_{typ}} \lambda$.)



SAMPLE CALCULATION:

$\mu = .4D$

LEVEL SPACING = .1 cm^{-1}

FIELD = 1 sv/cm

THE CALCULATION PLOTS POLARIZATION AGAINST THE TURN-ON RATE OF THE FIELD.

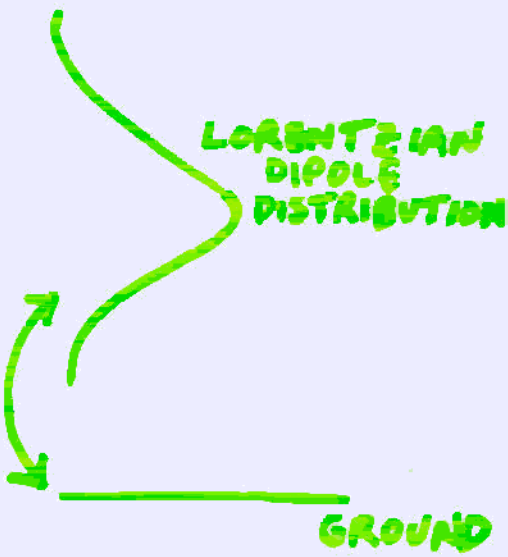
CLOSED-FORM SOLUTIONS:

CLOSED-FORMS OF SOLUTION (**) HAVE BEEN FOUND IN VARIOUS CASES. THE CLOSED-FORM SEPS IS KNOWN FOR A TWO-LEVEL SYSTEM, AND CLOSED-FORM EPS ARE KNOWN FOR:

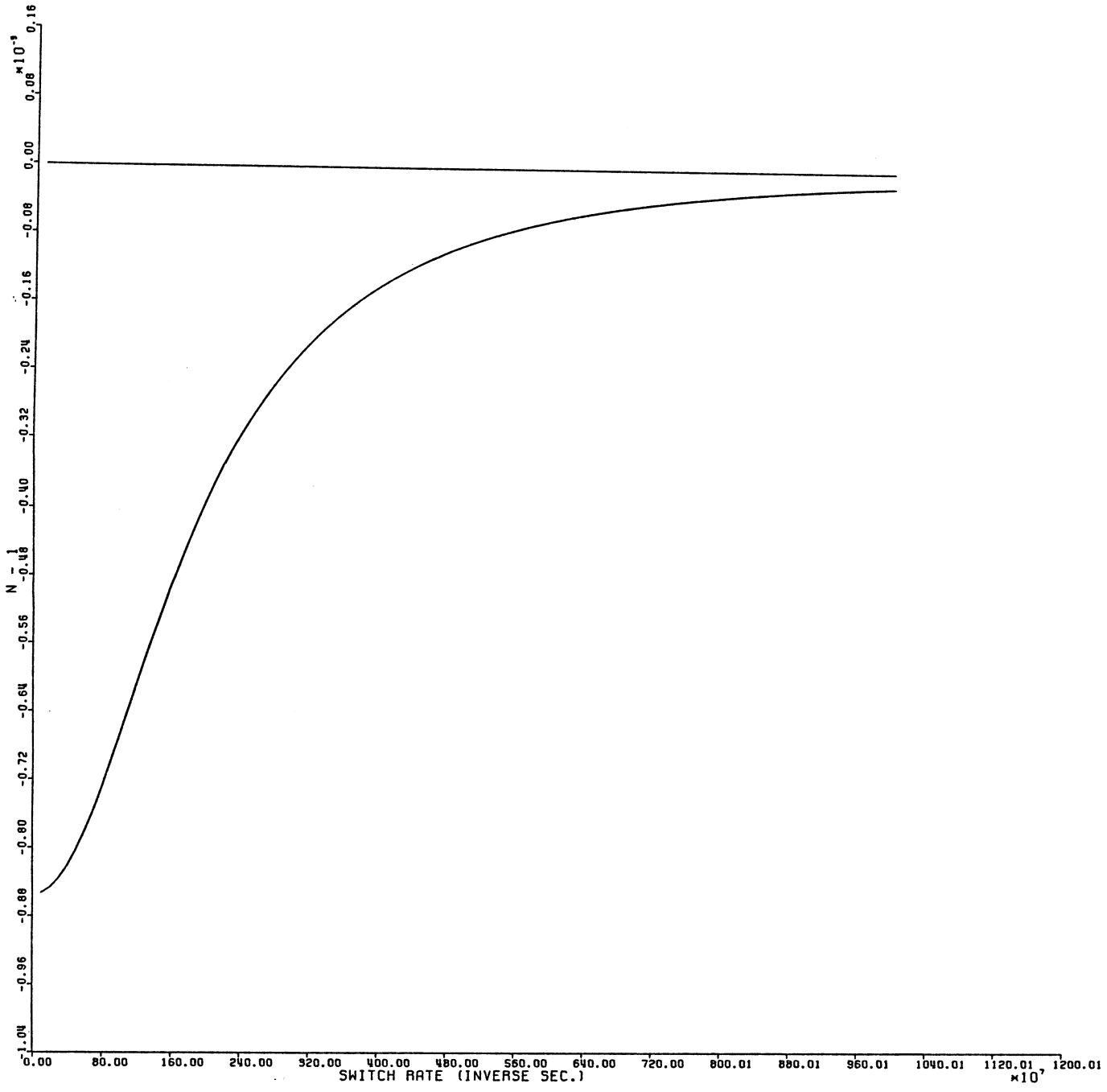
1) THE 2-LEVEL SYSTEM;
2) THE 3-LEVEL SYSTEM;

AND

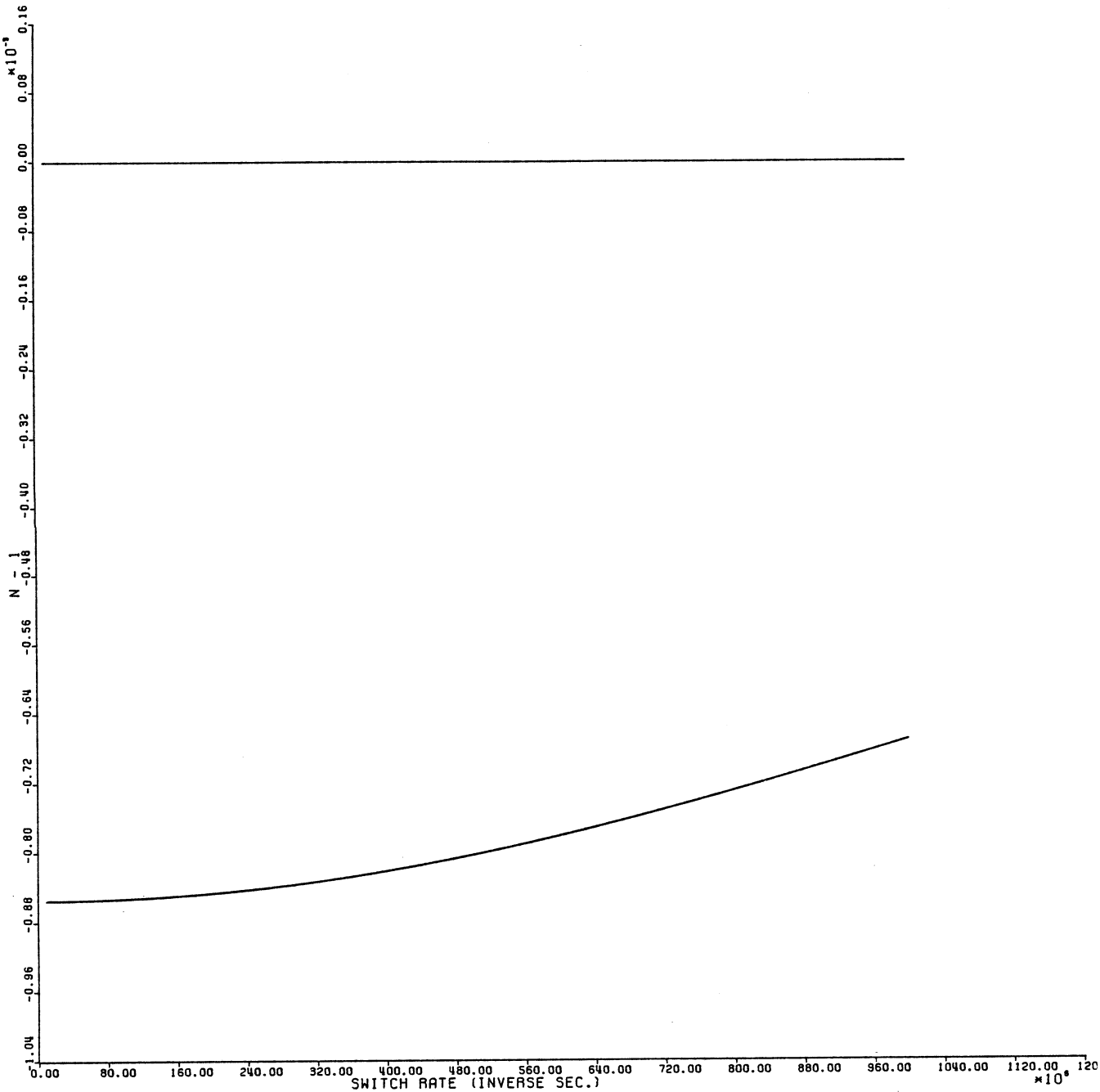
3) A SYSTEM WITH ONE DISTINGUISHED STATE AND A CONTINUUM OF STATES THAT CAN INTERACT WITH IT BY MEANS OF A LORENTZIAN DIPOLE DISTRIBUTION.



1 - 7 - 7 SYSTEM


N - 1
0.16
0.08
0.00
-0.08
-0.16
-0.24
-0.32
-0.40
-0.48
-0.56
-0.64
-0.72
-0.80
-0.88
-0.96
-1.04
×10⁻⁹
0.00
80.00
160.00
240.00
320.00
400.00
480.00
560.00
640.00
720.00
800.01
880.01
960.01
1040.01
1120.01
1200.01
SWITCH RATE (INVERSE SEC.)
×10⁷

1 - 7 - 7 SYSTEM


N - 1
*10⁻⁹
0.16
0.08
0.00
-0.08
-0.16
-0.24
-0.32
-0.40
-0.48
-0.56
-0.64
-0.72
-0.80
-0.88
-0.96
-1.04
0.00
80.00
160.00
240.00
320.00
400.00
480.00
560.00
640.00
720.00
800.00
880.00
960.00
1040.00
1120.00
120
SWITCH RATE (INVERSE SEC.)
*10⁶

ALSO: IT IS KNOWN THAT CLOSED-FORM EPS CAN BE WRITTEN FOR ALL (1,N) SYSTEMS (i.e., SYSTEMS WITH ONE GROUND STATE AND N UPPER LEVELS THAT CAN INTERACT ONLY WITH THE GROUND STATE).

SAMPLE CLOSED-FORM EPS:

CONSIDER A SYSTEM WITH ONE LOWER LEVEL AND A LORENTZIAN DISTRIBUTION OF UPPER LEVELS, AND WITH THE FOLLOWING PARAMETERS:

R.M.S. DIPOLE MATRIX ELEMENT = μ_{01}
HWHM OF LORENTZIAN = σ
FIELD AT $(t=0)$ = E_0
DETUNING OF FIELD FROM CENTER OF LORENTZIAN = s
TURN-ON RATE OF FIELD = λ.

THEN

$$\tau = \frac{\mu_{01} E_0}{2\hbar\lambda} e^{\lambda t} .$$

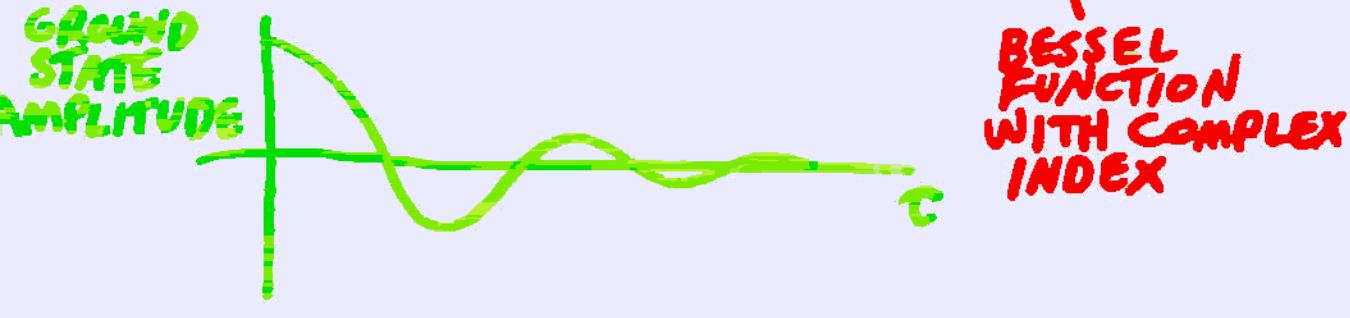
LETTING

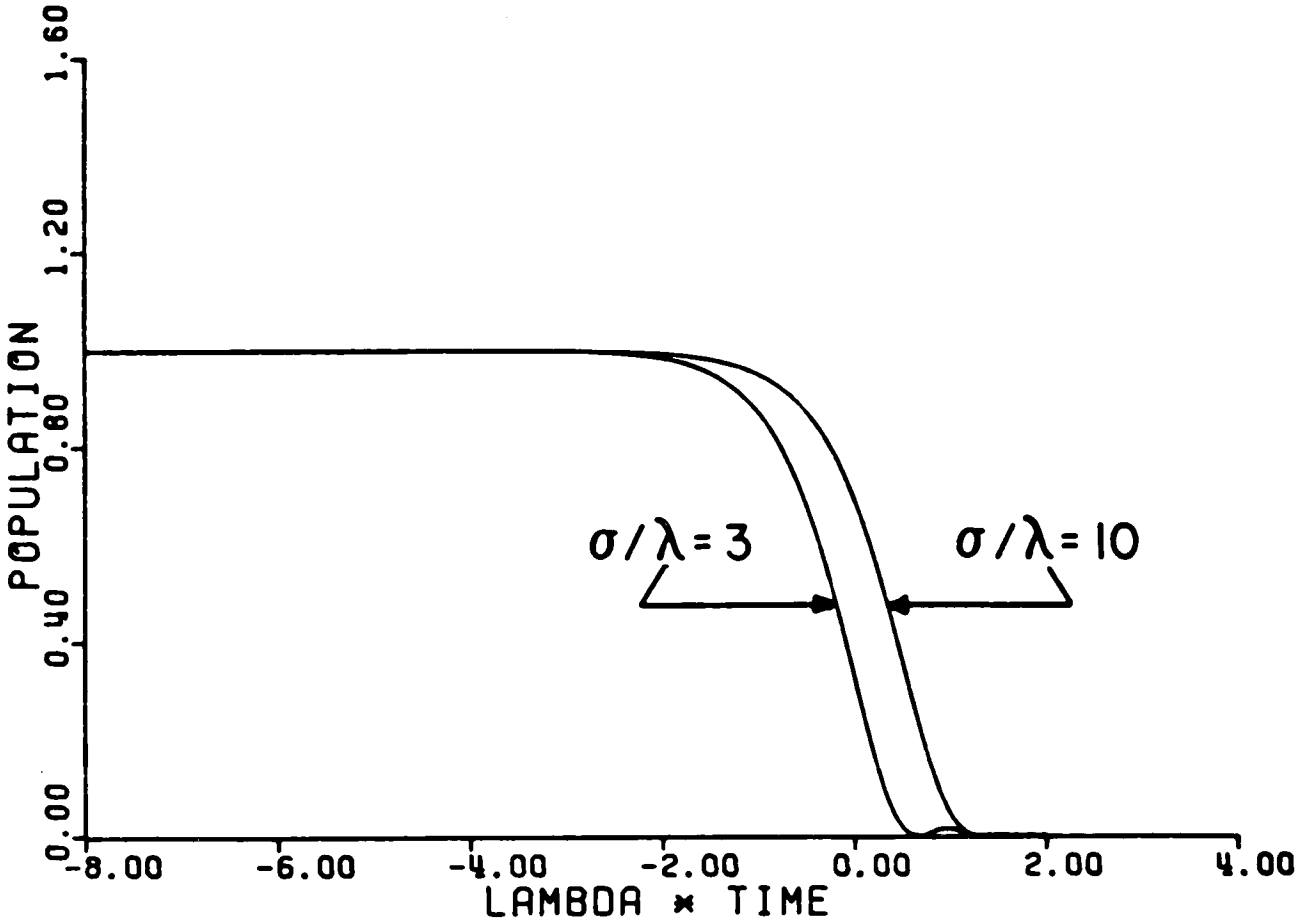
$$n = -\frac{1}{2}\left(1 + \frac{i}{\lambda}(s + i\sigma^2)\right),$$

THE CLOSED-FORM EPS IS

$$\langle v(t)\rangle_0 = \left(\begin{matrix}\text{GROUND-STATE}\\ \text{AMPLITUDE}\end{matrix}\right) = \left(\frac{2}{\tau}\right)^n n!\, J_n(\tau)$$

BESSEL FUNCTION WITH COMPLEX INDEX




POPULATION
1.60
1.20
0.80
0.40
0.00
-8.00
-6.00
-4.00
-2.00
0.00
2.00
4.00
LAMBDA * TIME
σ/λ = 3
σ/λ = 10

ADVANTAGES OF EPS TECHNIQUE

1) WHERE THE EPS (OR SEPS) IS BOTH APPLICABLE AND COMPUTATIONALLY PRACTICAL, IT IS FAR MORE EFFICIENT THAN NUMERICAL INTEGRATION.
2) THE EPS IS EASILY GENERALIZABLE TO DENSITY-MATRIX CALCULATIONS.
3) THE EPS GRADUATES SMOOTHLY BETWEEN THE SUDDEN AND ADIABATIC APPROXIMATIONS.
4) THE EPS COMPRESSES THE LONG (POSSIBLY INFINITE) HEAD OR TAIL OF A PULSE INTO A SHORT (FINITE) INTERVAL.
5) MANY CLOSED-FORM SOLUTIONS ARE KNOWN.
6) MANY ASYMPTOTIC RESULTS (GIVING POPULATIONS IN THE LIMIT $t \to \infty$ AS EXPLICIT FUNCTIONS OF TURN-ON TIME, DETUNING, ETC.) ARE KNOWN.
7) THE EPS (OR SEPS) IS APPLICABLE EVEN IN THE CASE OF A CONTINUOUS LEVEL-STRUCTURE.
8) THE COEFFICIENTS IN THE EPS SERIES DO NOT DEPEND ON E_0. FOR LARGER FIELDS, JUST EVALUATE AT LARGER t.

DISADVANTAGES

1) THE NUMERICAL CONVERGENCE OF THE EPS IS NOT AS GOOD FOR SLOW PULSES AS IT IS FOR FAST PULSES.
2) THE EPS CANNOT BE GENERALIZED FOR ARBITRARY PULSE SHAPES.